

JINS Workshop

Using Neutrons to Probe Structure and Dynamics in Biological Systems

April 8-10, 2002

Pollard Auditorium

Oak Ridge, Tennessee

April 8, 2002 *Morning – Lee Magid, Chair*

- 8:00** **Welcome and Announcements – Frank Harris and Michelle Buchanan**
- 8:15** **Overview of SNS and Its Central Lab Office Building – Thom Mason**
- 9:15** **Protons in Proteins: Are They There? – Dagmar Ringe**
- 10:15** **Break**
- 10:45** **Neutrons, Proteins, Membranes, Warm Water and a Pinch of Salt – Joe Zaccai**
- 11:45** **Lunch; Informal viewing of posters**

April 8, 2002 *Afternoon – Michelle Buchanan, Chair*

- 1:15** **Fundamentals of SANS from Biological Macromolecules – Susan Krueger**
- 2:15** **Small-Angle Scattering: Solutions In Protein Structural Analysis – Joanna Krueger**
- 2:45** **Break**
- 3:00** **Neutrons, Protons and Proteins – Dean Myles**
- 4:00** **Detergent Organization in Crystals of Monomeric Outer Membrane Phospholipase A – Harm Jan Snijder, K. H. Kalk, P. A. Timmins and B. W. Dijkstra**
- 4:30** **Center for Structural and Molecular Biology; Instrumentation at HFIR for Biology – Michelle Buchanan/Paul Butler**
- 5:15** **Poster Session**
- 6:30** **Cash Bar, Garden Plaza**
- 7:00** **Dinner, Garden Plaza Hotel**
Speaker – Jill Trewhella “Neutrons in Biology; Post Human Genome and September 11”

April 9, 2002 *Morning* – Mathias Lösche, Chair

- 8:15 ORAU Interest in Neutrons and Biology – Ron Townsend**
- 8:30 Neutrons: An Ideal Probe for Biological Materials – John Katsaras**
- 9:30 Determining the Structures of Peptides in Membranes Using Diffraction and MD Simulations – Steve White and Kalina Hristova**
- 10:00 Break**
- 10:30 Neutron Reflectivity from Biomimetic Membranes – David Vaknin**
- 11:30 The Structure of Organized Lipid Layers – Greg Smith**
- Noon Lunch; Informal viewing of posters**

April 9, 2002 *Afternoon* – Doug Tobias, Chair

- 1:00 Methods of Inelastic Neutron Scattering for Biological Systems – Dan Neumann**
- 2:00 Measuring the Dynamic Behavior of a Protein with Quasielastic Neutron Scattering – Adam Pivovar**
- 2:30 Biomolecules Studied with Neutron Spectroscopy: The Impact of Conformational Dynamics on Function and Stability of Proteins – Joerg Fitter, KFA Juelich**
- 3:00 Break**
- 3:30 Interpretation of Neutron Scattering Data on Biomolecular Structure and Dynamics Using Molecular Modeling and Simulation – Doug Tobias**
- 4:30 Session on Details of Instrumentation for Biology at SNS – Ken Herwig, John Ankner, Christina Hoffmann**
- 5:15 Adjourn**
- 6:00 Depart for dinner and entertainment, Museum of Appalachia**

April 10, 2002 *Morning*

- 8:15 Joint Institute for Neutron Sciences – Lee Magid**
- 8:30 Center for Nanophase Materials Sciences – Michelle Buchanan**
- 9:00 ORNL support facilities for users of SNS/HFIR – Michelle Buchanan**
- 9:15 Organizer – Ken Herwig**
Discussion facilitated by Ken Herwig, Paul Butler, Joanna Krueger, Xun-Li Wang
- **User community's needs for supporting facilities to optimize use of SNS, HFIR and CNMS**
 - **Additional instruments needed for biology**
 - **Building the neutron scattering community in the biological sciences**
 - **Next steps – identification of flag carriers and their follow-on activities**
- 11:45 Summation – Ron Townsend/Michelle Buchanan**

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